NUMERICAL CALCULATION OF FRACTIONAL DERIVATIVES OF NON-SMOOTH DATA

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Abstract

This paper addresses the calculation of fractional derivatives of fractional order for non-smooth data. The noise is avoided by adopting an optimization formulation using genetic algorithms (GA). Given the flexibility of the evolutionary schemes it is established a hierarchical GA composed by a series of two GAs, each one with having a distinct fitness function.

Key words

Fractional calculus, numerical differentiation, genetic algorithms.

1 Introduction

Fractional calculus (FC) deals with the generalization of integrals and derivatives to a non-integer, or even complex, order [Bagley, et al. 1983; Miller, et al. 1993; Oldham, et al., 1974; Ross, 1977; Samko, et al. 1993]. FC encompasses a wide range of potential fields of application by bringing into broader paradigm concepts of physics, chemistry and engineering [Machado, 1997; Machado, 2001; Mainardi, 1996; Oustaloup, 1991; Podlubny, 1999]. Nevertheless, until recently, FC was an 'unknown' mathematical tool for the applied sciences, being the present day interest motivated by the developments in the areas of nonlinear dynamics, chaos and modeling.

One of the reasons for this state of affairs is the lack of a simple interpretation for a fractional order derivative. In fact, while for the integer-order case we have a common geometric concept in the fractional-order case we have problems in finding a clear and comprehensive reasoning scheme. Several researchers proposed different approaches for the interpretation of fractional-order integrals and derivatives, but the fact is that a final paradigm is not yet well established [Adda, 1997; Machado, 2003; Moshrefi-Torbati et al. 1998; Nigmatullin, 1992; Podlubny, 2002; Rutman, 1994; Stanislavsky, 2004; Tatom, 1995; Yu, et al. 1997].

A second reason for the difficulties in applying FC is due to the higher complexity of algorithms for the calculation of fractional derivatives and integrals. The generalization of the integrodifferential operator requires the adoption of approximations based on series or rational fraction expansions [Oustaloup, 1991; Machado, 1997]. While the main volume of contributions has focused in getting the best approximation scheme, the problem of its calculation for real data was not yet tackled. In fact, besides the quality of the approximation, two aspects must be considered in the calculation of fractional derivatives and integrals, namely the computational load and the effect of noise. The first aspect poses a small impact in today's computing systems, but the second remains to be investigated.

The problem of calculating integer-order derivatives for noisy data is well known. For avoiding the emergence of high amplitude peaks the classical approach consists in adopting polynomials on increasing order, or a plethora of distinct types of low-pass filters, that somehow smooth the data [Chartrand, 2005; Li, 2005]. However, it was verified that, in many cases, those measures are not successful. Bearing these facts in mind, more recently it was recognized that the problem was ill posed and that an inverse formulation, incorporating an optimization scheme, was the best strategy.

In this line of thought, this paper addresses the calculation of fractional derivatives of fractional order for non-smooth data, and is organized as follows. Section 2 introduces the calculation of fractional derivatives for ideal data, the problem of noise and the formulation of the inverse problem, and the optimization scheme based on genetic algorithms. Section 3 presents a set of experiments that demonstrate the effectiveness of the proposed method. Finally, section 4 outlines the main conclusions.

2 Problem Formulation and Adopted Tools

2.1 Fractional Derivatives

Since the foundation of the differential calculus the generalization of the concept of derivative and integral to a non-integer order α has been the subject of several approaches such as the Riemann-Liouville, Grünwald-Letnikov, Caputo and, based on transforms, the Fourier/Laplace definitions.

From the discrete-time point of view the Grünwald-Letnikov definition seems more attractive and, consequently will be adopted in the sequel.

Based on the concept of fractional differential of order α, the Grünwald-Letnikov definition of a derivative of fractional order α of the signal $x(t)$, $D^{\alpha}x(t)$, consists in the expression:

$$D^{\alpha}x(t)=\lim_{h\to 0}\frac{1}{h^{\alpha}}\sum_{k=0}^{\infty}\frac{(-1)^{k}\Gamma(\alpha+1)x(t-kh)}{\Gamma(k+1)\Gamma(\alpha-k+1)} \tag{1}$$

where Γ is the gamma function and h is the time increment. This formulation inspires a discrete-time calculation algorithm, based on the approximation of the time increment h through the sampling period T, yielding the equation in the z domain:

$$D^{\alpha}X(z)\approx\left[\frac{1}{T^{\alpha}}\sum_{k=0}^{\infty}\frac{(-1)^{k}\Gamma(\alpha+1)}{k!\,\Gamma(\alpha-k+1)}z^{-k}\right]X(z) \tag{2}$$

The implementation of expression (2) corresponds to a r-term truncated series given by:

$$D^{\alpha}X(z)\approx\left[\frac{1}{T^{\alpha}}\sum_{k=0}^{r}\frac{(-1)^{k}\Gamma(\alpha+1)}{k!\,\Gamma(\alpha-k+1)}z^{-k}\right]X(z) \tag{3}$$

This series can be implemented by a rational fraction expansion which leads to a superior compromise in what concerns the number of terms versus the quality of the approximation. Nevertheless, since the study focuses mainly the problem of noise, the simple series approximation will be adopted.

2.2 Calculation of Derivatives of Noisy Data

In many scientific applications it is necessary to calculate the derivative of numerical data. Classical finite-difference approximations amplify greatly any noise present in the data. Data denoising, before or after differentiating, does not generally give satisfactory results. A method that leads to good results consists in the regularization of the differentiation process itself. This guarantees that the computed derivative will have some degree of regularity, to an extent that is under control by adjusting parameters. A common framework for the regularization [Ahnert, et al. 2006; Chartrand, 2005; Knowles, 1995; Le, et al. 2007] corresponds to the formulation of the inverse problem. In this perspective, $u(t)$, the derivative of a function $f(t)$ over the interval $t\in[0,L]$, is the minimizer of the functional:

$$F(u)=aR\{u\}+S\{A[u]-f\} \tag{4}$$

where $R\{u\}$ is a regularization term that penalizes irregularity in $u(t)$, $A[u(t)]=\int_0^t u\,dt$ is the operator of antidifferentiation, $S\{A[u]-f\}$ is a data similarity term that penalizes discrepancy between $A[u]$ and f, and $a\in\Re^{+}$ is a regularization parameter that controls the balance between the two terms.

The regularization and similarity terms, $R\{\ \}$ and $S\{\ \}$, adopt often the squared L^2 norm. Therefore, it is considered that the total-variation regularization and the computation of the derivative of f over the interval $[0, L]$ is the minimizer of the functional:

$$F(u)=a\int_0^L \dot{u}^2dt+\int_0^L\{A[u]-f\}^2\,dt \tag{5}$$

where for convenience is assumed that $f(0)=0$ which, in practice consists in subtracting $f(0)$ from $f(t)$.

A simple approach to minimizing (5) is gradient descent as described in [Chartrand, 2005]. However, in the present study it will be adopted a different optimization technique based on genetic algorithms (GAs) due to its superior flexibility. In fact, the standard numerical optimization has difficulties in achieving an adequate compromise between the terms $R\{\ \}$ and $S\{\ \}$. The optimization requires several attempts, with distinct values of the regularization parameter a, and often we verify that there is no good tuning. Therefore, in the next sub-section we adopt a hierarchical GA with two simple GAs in series, each one optimizing a separate term.

2.3 Optimization with Genetic Algorithms

A GA is a search technique used in computing to find exact or approximate solutions to optimization and search problems. GAs are simulated in a computing system, and consist in a population of representations of candidate solutions, of an optimization problem, that evolve toward better solutions.

Once the genetic representation and the fitness function are defined, the GA proceeds to initialize a population of solutions randomly, and then to improve it through the repetitive application of mutation, crossover, inversion and selection operators.

The evolution usually starts from a population of randomly generated individuals. In each generation, not only the fitness of every individual in the population is evaluated, but also several individuals are stochastically selected from the current population and modified to form a new population. The new population is then used in the next iteration of the algorithm. The GA terminates when either a maximum number of generations has been produced, or a satisfactory fitness level has been reached.

During the successive generation, a part or the totality of the population is selected to breed a new generation. Individual solutions are selected through a fitness-based process, where fitter solutions (measured by a fitness function) are usually more likely to be selected. The pseudo-code of the GA is:

```
1. Choose the initial population
2. Evaluate the fitness of each
individual in the population
3. Repeat
  3.1. Select best-ranking
  individuals to reproduce
  3.2. Breed new generation
  through crossover and mutation
  and give birth to offspring
  3.3. Evaluate the fitness of
  the offspring individuals
  3.4. Replace the worst ranked
  part of population with
  offspring
4. Until termination
```

In the present article it also used the common technique of elitism which is the process of selecting the better individuals to form the parents in the offspring generation.

As mentioned in the previous subsection the minimization of $F(u)$ in expression (5) poses problem of establishing a compromise between the terms $R\{\ \}$ and $S\{\ \}$. Therefore, given the flexibility of the evolutionary schemes it was established a hierarchical GA composed by a series of two GAs, that is $GA_{12} = \{GA_1 + GA_2\}$, each one with having a distinct fitness function corresponding to:

$$F_1(u) = R\{u\} = \int_0^L \dot{u}^2 dt \tag{6a}$$

$$F_2(u) = S\{A[u] - f\} = \int_0^L \{A[u] - f\}^2 dt \tag{6b}$$

The GA population is constituted by a series of candidate values $\mathbf{U} = [u_i]$, established at the discrete sampling points $\mathbf{T} = [t_i]$, $i = 0, \cdots, n$, and the evolution consists in a loop of iterations of the GA according with the pseudo-code:

```
1. Choose the initial population
2. Repeat
  2.1. Execute N1 iterations of
  GA1 with fitness function F1
  2.2. Execute N2 iterations of
  GA2 with fitness function F2
3. Until termination
```

where termination occurs for a total number of iterations $N_{12} \sim (N_1 + N_2)$.

3 Fractional Differentiation of Noisy Data

In this section we evaluate the proposed technique in the numerical evaluation of a fractional derivative of a function corrupted by additive noise.

In the experiments the GA_{12} adopts $N_1 = N_2 = 1$, a population of $P = 100$ individuals, mutation probability $p_m = 0.1$, single point crossover and reproduction within all population considering elitism. The number of sampling points $n = 30$, the function $f(t) = t$ defined over the interval $t \in [0,1]$, and additive noise given by a uniform probability density function in the interval $[-X, +X]$.

Since the global performance is sensitive to the number of iterations and the amplitude of the noise, we investigate the GA_{12} performance for $N_{12} = \{10^3, 5\ 10^3, 10^4, 5\ 10^4, 10^5\}$ and $X = \{0.0, 5.0\ 10^{-3}, 10^{-2}, 5.0\ 10^{-2}, 10^{-1}\}$.

It is considered the evaluation of a derivative of order $\alpha = 1/2$ through the series approximation (3) where $T = 1/n$ and $r = n = 30$ in order to avoid truncation errors. For initialization matters it is considered $f(t) = 0$, $t < 0$, and, consequently, that additive noise affects $f(t)$ only in the interval $t \in [0,1]$. Moreover, due to the stochastic nature of the evolutionary schemes, the experiments are repeated for $N_T = 10$ cases with different initial random GA populations.

Figure 1 depicts the results of the new computational scheme for the case of $f(t)$ without any noise (*i.e.*, $X = 0.0$) and $N_{12} = 10^3$ and $N_{12} = 10^5$.

We verify that the GA has a poor performance for a low number of iterations, but it captures adequately the derivative when a high number of iterations are executed leading to a chart very close to the theoretical value of $D^{1/2}t = 2\sqrt{t/\pi}$. The slow GA convergence is, in fact, due to the requirement posed by the series of the two distinct fitness functions.

Figure 2 shows the corresponding result for an additive noise with amplitude $X = 0.01$ and $N_{12} = 10^4$ and $N_{12} = 10^5$ iterations. We verify that noise poses more stringent requirements but that, after a sufficient number of iterations, we get good results.

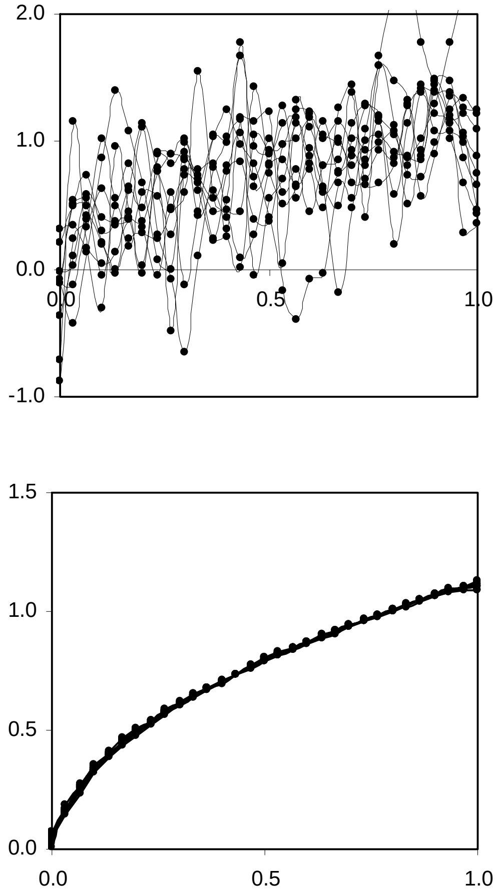

Figure 1. Chart of $D^{1/2}t$, $0 \le t \le 1$, $X = 0.0$, for $N_{12} = 10^3$ and $N_{12} = 10^5$ ($n = 30$, $N_T = 10$).

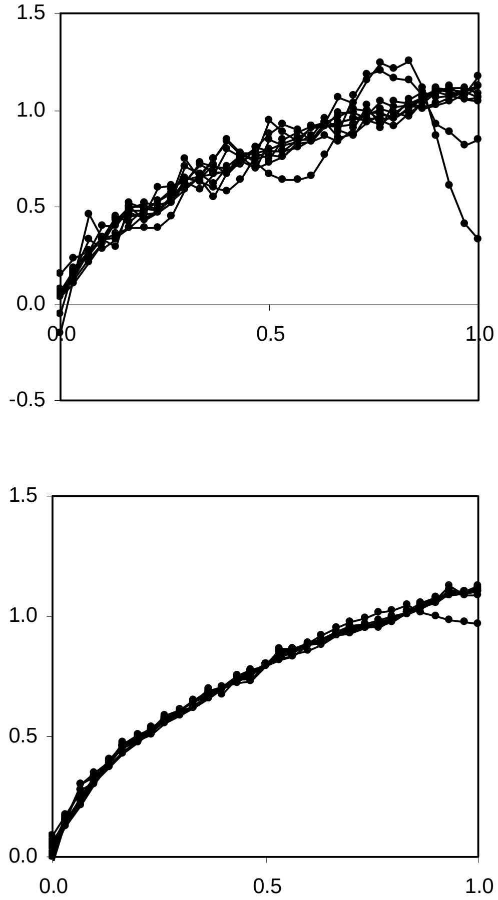

Figure 2. Chart of $D^{1/2}t$, $0 \le t \le 1$, $X = 0.01$, for $N_{12} = 10^4$ and $N_{12} = 10^5$ ($n = 30$, $N_T = 10$).

4 Conclusions

The recent advances in fractional calculus point towards important developments in the application of this mathematical concept. During the last years were proposed several algorithms for the approximate calculation of fractional derivatives and integrals. Nevertheless, the real case of data with noise was somewhat overlooked. In this paper it was proposed a new method based on evolutionary concepts for the calculation of fractional derivatives. In this line of thought, it was introduced an optimization formulation and a hierarchical genetic algorithm, consisting in a series of two GAs, capable of handling the distinct requirements posed by the derivative calculation and the noise elimination. The results demonstrate the excellent performance, namely the convergence and the robustness for high levels of noise. While the study addressed an off-line calculation strategy, the results suggest that an on-line calculation may be feasible when optimizing the evolutionary scheme.

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